

APPENDIX 1

Program for Baselining, Normalizing, Interpolating Then Calculating Spectral Overlap Integrals

5 C This program has a non-standard DO WHILE loop

10 INTEGER NPTS, NMAX, ROWS, ITER
INTEGER EOF1, FLERR1, FLERR2
INTEGER EOF2, FLERR3, FLERR4
15 INTEGER EOF3, FLERR5, FLERR6
INTEGER FLERR7
INTEGER i,j
CHARACTER*30 fname1, fname2, fname3, fname4
CHARACTER*30 fname5, fname6, fname7
PARAMETER(NMAX=3500, LAMDA=601)
REAL x,xx1 (NMAX),yy1 (NMAX),INTERV1
REAL xx2 (NMAX),yy2 (NMAX),INTERV2
20 REAL xx3 (NMAX),yy3 (NMAX),INTERV3
REAL y1 (NMAX), y12 (NMAX), y13 (NMAX), yc (NMAX)
REAL area
CHARACTER*1 SUBSTR, INITAR, LIGHT, INTMED

25 FLERR1=0
FLERR2=0
FLERR3=0
FLERR4=0
FLERR5=0
FLERR6=0
30 FLERR7=0
EOF1=0
EOF2=0
EOF3=0
INTERV1=0
35 INTERV2=0
INTERV3=0
area=0

40 write(*,*) 'Do you wish to output intermediate files? (Y/N)'
read(*, '(A)') INTMED

45 write(*,*) 'Do you wish to process a substrate file? (Y/N)'
read(*, '(A)') SUBSTR

45 IF ((SUBSTR.EQ.'Y') .OR. (SUBSTR.EQ.'y')) THEN

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ITER=0
do 5 ITER=1, NMAX
    xx1 (ITER)=0
    yy1 (ITER)=0
    yi1 (ITER)=0
5      continue

10      write(*,*) 'Enter the name of the input substrate file:'
         read(*, '(A)') fname1

15      open
         (UNIT=11,FILE=fname1,STATUS='OLD',IOSTAT=FLERR1,E
         RR=101)
ROWS=0

20      do while ((EOF1.EQ.0) .AND. (ROWS.LT.NMAX))
         ROWS=ROWS+1
         Read (11,* ,IOSTAT=EOF1) xx1 (ROWS), yy1 (ROWS)
      end do

25      close (UNIT=11)
NPTS=0

30      IF (EOF1.NE.0) THEN
         NPTS=ROWS-1
         write(* ,'(I4,1X,A12)') NPTS, 'points read.'
      ELSE
         NPTS=ROWS
         write(* ,'(A28, I4, A12)') 'Too many data points! First',
+                                         NMAX, ' points read...'
      END IF

35      call baseln(yy1,NPTS)

40      IF ((INTMED.EQ.'Y') .OR. (INTMED.EQ.'y')) THEN
         write(*,*) 'Enter the name of the output substrate file:'
         read(*, '(A)') fname2
         open
         (UNIT=12,FILE=fname2,STATUS='NEW',IOSTAT=FLERR2,
         ERR=102)

45      write(*,*) 'Writing data...'

END IF

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x=0
i=0
j=0
5
do 12 i=1, LAMDA

      x= (i-1)+200

10      call locate(xx1,NPTS,x,j)

      if ((j.eq.0). OR. (j.eq.NPTS)) then
          INTERV1=0
      else
          INTERV1= ((yy1(j+1)-yy1(j)) / (xx1(j+1) - xx1(j))) *
15          (x-xx1(j))
          +
          +yy1(j)

      end if

      yi1 (i)=INTERV1

      IF ((INTMED.EQ.'Y') .OR. (INTMED.EQ.'y')) THEN

          if ((j.eq.0) .OR. (j.eq.NPTS)) then
              GO TO 12
          else
              write(12,'(1x, f7.2,i6,3f12.2)')x,j,xx1(j),xx1(j+1),
+                  INTERV1
          endif
30

      END IF

      12      continue
      IF ((INTMED.EQ.'Y') .OR. (INTMED.EQ.'y')) THEN
          close (UNIT=12)

      END IF
40
      ELSE
          ITER=0
          do 14 ITER=1, LAMDA
              yi1 (ITER)=1
45          14          continue

      ENDIF

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      write(*,*) 'Do you wish to process an initiator file? (Y/N)'
      read(*,'(A)') INITAR

      5      IF ((INITAR.EQ.'Y') .OR. (INITAR.EQ.'y')) THEN

              ITER=0

10      do 15 ITER=1,NMAX
              xx2 (ITER) =0
              yy2 (ITER) =0
              yi2 (ITER) =0
15      continue

15      write(*,*) 'Enter the name of the initiator file:'
      read(*,'(A)') fname3

20      open
              (UNIT=13,FILE=fname3,STATUS='OLD',IOSTAT=FLERR3,
              ERR=103)

25      ROWS=0

      do while ((EOF2.EQ.0) .AND. (ROWS.LT.NMAX))
              ROWS=ROWS+1
              read(13,*,IOSTAT=EOF2) xx2 (ROWS), yy2 (ROWS)
      end do

30      close (UNIT=13)

35      NPTS=0

      IF (EOF2.NE.0) THEN
              NPTS=ROWS-1
              write(*,1(14,1X,A12)) NPTS,'points read.'
      ELSE
              NPTS=ROWS
              write (*,'(A28,I4,A12)') 'Too many data points! First ',
+                                         'NMAX,' points read...
      END IF
      call baseln (yy2,NPTS)

40      IF ((INTMED.EQ.'Y').OR. (INTMED.EQ.'y')) THEN

              write(*,*) 'Enter the name of the output initiator file:'
              read(*,'(A)') fname4

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          open
(UNIT=14,FILE=fname4,STATUS='NEW',IOSTAT=FLERR4,
ERR=104)

5      write(*,*) 'Writing data...'

END IF
x=0
i=0
10     j=0

do 22 i=1,LAMDA
      x= (i-1)+200

15     call locate (xx2,NPTS,x,j)
if ((j.eq.0).OR. (j.eq.NPTS)) then
      INTERV2=0
      else
      INTERV2= ((yy2(j+1)-yy2(j)) / (xx2(j+1) - xx2
(j))) * (x-xx2 (j))
      +
      +yy2 (j)
      end if
      yi2 (i)=INTERV2
      IF ((INTMED.EQ.'Y') .OR. (INTMED.EQ.'y')) THEN
      if ((j.eq.0) .OR. (j.eq.NPTS)) then
          GO TO 22
      else
          write(14,'(1x,f7.2,i6,3f12.2)') x, j, xx2
30      (j),xx2 (j+1),
      +
          INTERV2
      endif
      END IF

35     END IF

22     continue

40     IF ((INTMED.EQ.'Y').OR. (INTMED.EQ.'y')) THEN
      close (UNIT=14)

END IF
ELSE
45     ITER=0

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do 24 ITER=1,LAMDA
    yi2 (ITER)=1
24        continue

5        ENDIF
write(*,*) 'Do you wish to process a light source file? (Y/N)'
read(*,')(A)') LIGHT

10       IF ((LIGHT.EQ.'Y').OR. (LIGHT.EQ.'y')) THEN
        ITER=0
        do 25 ITER=1,NMAX
            xx3 (ITER) =0
            yy3 (ITER) =0
            yi3 (ITER)=0
15        25        continue

        write(*,*) 'Enter the name of the light source file:'
        read(*,')(A)') fname5

        open
        (UNIT=15,FILE=fname5,STATUS='OLD',IOSTAT=FLERR5,
        ERR=105)

        ROWS=0

        do while ((EOF3.EQ.0) .AND. (ROWS.LT.NMAX))
            ROWS=ROWS+1
            read(15,*,IOSTAT=EOF3) xx3 (ROWS), yy3 (ROWS)
        end do
30

        close (UNIT=15)

        NPTS=0
        IF (EOF3.NE.0) THEN
            NPTS=ROWS-1
            write(*,1 (14,1X,A12)) NPTS, 'points read.'
        ELSE
            NPTS=ROWS
            write (*,')(A28,I4,A12)') 'Too many data points! First ',
40        +                                NMAX, ' points read...'
            END IF

            call norm (yy3,NPTS)

45        IF ((INTMED.EQ.'Y').OR. (INTMED.EQ.'y')) THEN

            write(*,*) 'Enter the name of the light source output file:'

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read(*, '(A)') fname6
 open
 (UNIT=16,FILE=fname6,STATUS='NEW',IOSTAT=FLERR6,
 ERR=106)
 5
 write(*,*) 'Writing data...'
 END IF
 x=0
 10 i=0
 j=0
 do 32 i=1,LAMDA
 x=(i-1)+200
 15 call locate (xx3,NPTS,x,j)
 if ((j.eq.0) .OR. (j.eq.NPTS)) then
 INTERV3=0
 else
 INTERV3= ((yy3(j+1) - yy3(j)) / (xx3(j+1) -
 xx3(j))) * (x-xx3 (j))
 +
 end if
 yi3 (i)=INTERV3
 IF ((INTMED.EQ.'Y') .OR. (INTMED.EQ.'y')) THEN
 if ((j.eq.0).OR. (j.eq.NPTS)) then
 GO TO 32
 else
 30 write(16,'(1x,f7.2,i6,3f12.2)') x,j,xx3 (j),xx3 (j+1),
 + INTERV3
 endif
 END IF
 35 32 continue
 IF ((INTMED.EQ.'Y') .OR. (INTMED.EQ.'y')) THEN
 close (UNIT=16)
 40 END IF
 ELSE
 ITER=0
 45 do 34 ITER=1,LAMDA
 yi3 (ITER)-1
 34 continue

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ENDIF

ITER=0

DO 40 ITER=1,LAMDA
    yc (ITER)=0
40        CONTINUE

DO 55 i=1,LAMDA
    yc (i) -yi1 (i)*yi2 (i)*yi3 (i)
55        CONTINUE

write(*,*) 'Enter the filename for cumulative data:'
read (*,')(A)') fname7
open
(UNIT=17,FILE=fname7,STATUS='NEW',IOSTAT=FLERR7,
ERR=107)
write(*,*) 'Writing data...'

CALL integ (yc,LAMDA,area)

write(*,'(1X,A26,A11,F12.6)') 'The area under the product',
+'curve is:',area

write(17,'(1X,A26,A11,F12.6)') 'The area under the product',
+' curve is: ',area

DO 60 i=1,LAMDA
    x=(i-1)+200
    write(17,'(1X,F6.1,2F11.2,F11.4,E15.6)') x,yi1 (i),yi2
(i),
+                    yi3 (i) ,yc (i)
60        CONTINUE

close (UNIT=17)

101 IF (FLERR1 .NE. 0) THEN
    write(*,*) 'Unable to open substrate file!'
END IF

102 IF (FLERR2 .NE. 0) THEN
    write(*,*) 'Unable to create substrate output file!'
END IF

103 IF (FLERR3 .NE. 0) THEN
    write(*,*) 'Unable to open initiator file!'
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END IF

104  IF (FLERR4 .NE. 0) THEN
      write(*,*) 'Unable to create initiator output file!'
END IF

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105  IF (FLERR6 .NE. 0) THEN
      write(*,*) 'Unable to open light source file!'
END IF

10

106  IF (FLERR6 .NE. 0) THEN
      write(*,*) 'Unable to create light source output file!'
END IF

15

107  IF (FLERR7 .NE. 0) THEN
      write(*,*) 'Unable to create cumulative output file!'
END IF

20

write(*,*) 'Program exiting normally...'

END

SUBROUTINE locate (xx,n,x,j)
INTEGER j,n
REAL x,xx (n)
INTEGER j1,jm,ju
J1=0
ju=n+1
10      if (ju-j1.gt.1) then
        jm= (ju+j1)/2
        if ((xx (n).ge.xx (1)) .eqv. (x.ge.xx (jm))) then
          j1=j m
        else
          ju=jm
        endif
35      goto 10
      endif
      if (x.eq.xx (1))then
        j=1
40      else if (x.eq.xx(n))then
        j=n-1
      else
        j=j1
      endif
45      return END

SUBROUTINE baseln (yy,N)

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      INTEGER N, i
      REAL yy (N), minno, temp

      5      minno=yy (1)
             i=0
             temp=0

      DO 10 i=2,N
      10      IF (yy (i) .LT. minno) THEN
                  minno=yy (i)
              END IF
      10      CONTINUE

      15      i=0

      DO 20 i=1,N
      20      temp=yy (i)-minno
                  yy (i)=temp
      20      CONTINUE

      END

      SUBROUTINE norm (yy,N)

      INTEGER N, i
      REAL yy (N),maxno,temp

      maxno=yy (1)
      i=0
      temp=0

      DO 5 i=2,N
      5      IF (yy(i).GT.maxno) THEN
                  maxno=yy (i)
              END IF
      5      CONTINUE

      i=0

      DO 10, i=1,N
      10      temp=yy (i)/maxno
                  yy (i)=temp
      10      CONTINUE

      END

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SUBROUTINE integ (yy,N,area)

      INTEGER N,i
      REAL yy (N),sum,area
      5
      i=0
      sum=0
      area=0
      10      DO 10 i=1,N-1
              sum=sum+ (yy(i)+yy (i+1))*0.5
      10      CONTINUE
      15      area=sum/100000
      END

```

APPENDIX 2

Program to create uniformly spaced csv data from unevenly spaced tabular data

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```
#include <stdio.h>
#include <stdlib.h>
#include <math.h>

#define NMAX 3501
#define STRMAX 151
#define FNMAX 81
#define OUTPTS 801

void locate(float xx[], unsigned long n, float x, unsigned long *j);
void norm(float xx[], unsigned long int n);
void baseline(float xx[], unsigned long int n);

int main()
{
    char fnamein(FNMAX), string[STRMAX], *str, ptr,
    fnameout[FNMAX], another;
    float xdata(NMAX), ydata[NMAX], xinter[OUTPTS+1],
    yinter[OUTPTS+1];
    unsigned long int index, i, j;
    int choice;
    FILE *fpin, *fpout;

    another = 'Y';

    do {
        for (i = 0; i <= NMAX-1; i++) {
            xdata [i] = 0;
            ydata [i] = 0;
        };
        for (i = 0; i <= OUTPTS; i++) {
            xinter [i] = 0;
            yinter (i) = 0;
        };
        printf("Enter name of the input file (80 chars max, no spaces): ");
        scanf("%s", fnamein);

        printf("File name is %s\n", fnamein);

        fpin = fopen(fnamein,"r");

        if (fpin == NULL) {
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        printf("Cannot open %s\n", fnamein);
        exit(1);
    };

5      index = 1;

    while (1) {
        str_ptr = fgets(string, STRMAX-l, fpin);
        if(str_ptr == NULL)
            break;
        if (index == NMAX)
            break;
        sscanf(string, "%f %f", &xdata [index] , &ydata [index]);
        index++;
    };

15     fclose (fpin);

    if((index == NMAX) && (str_ptr != NULL)) {
        index--;
        printf("Too many data points! Using first %d points
only...\n",index);
    }
    else {
        index--;
        printf("%d points read...\n",index);
    };

20     printf("\nEnter option for data processing\n");
    printf("1: Normalize the data after interpolation\n");
    printf("2: Baseline the data after interpolation\n");
    printf("3: First interpolate, then baseline and finally ");
    printf("normalize the data\n");
    printf("4: Simply interpolate the data\n");
    printf("5: Simply normalize the data\n");
    printf("6: Simply baseline the data\n");
    printf("or\n");
    printf("0: to exit the program without any data processing\n");
    printf("\nEnter option (0-6): ");
40     scanf("%d",&choice);

    if (choice == 0)
        exit(2);

45     printf("\nEnter name of the output file (80 chars max, no spaces): ");
    scanf("%s", fnameout);

    printf("File name is %s\n", fnameout);

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fpout = fopen(fnameout,"w");

5      if (fpout == NULL) {
          printf("Cannot open %s\n",fnameout);
          exit(3);
      };

10     for(i = 1; i <= OUTPTS; i++) {
          xinter[i] = 200+((float)i-1);
          locate(xdata,index,xinter[i],&j);
          if ((j == 0) || (j == index))
              yinter[i] = 0;
          else
15          yinter[i] = (xinter[i] -xdata[j]) * ((ydata[j+1] -ydata[j]) /
              (xdata[j+1] -xdata[j])) +ydata[j];
      };

20     if ((choice == 2) || (choice == 3)) {
          baseline(yinter,OUTPTS);
      };

25     if (choice == 6) {
          baseline(ydata,index);
      };

30     if ((choice == 1) || (choice == 3)) {
          norm(yinter,OUTPTS);
      };

35     if (choice == 5) {
          norm(ydata,index);
      };

40     if ((choice >= 1) && (choice <= 4)) {
          for (i = 1; i <= OUTPTS-1; i++) {
              fprintf(fpout,"%13.5E, ",yinter[i]);
          };
          fprintf(fpout,"%13.5E\n",yinter[OUTPTS]);
      };
45     else
          if ((choice == 5) || (choice == 6)) {
              for (i = 1; i <= index-1; i++)
                  fprintf(fpout,"%13.5E, ",ydata[i]);
              };
              fprintf(fpout,"%13.5E\n",ydata[index]);
      };

fclose(fpout);

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printf("File %s written.\n\n",fnameout);
printf("Process another file (Y/y/N/n)?: ");
scanf("%ls",&another);
} while (another == 'Y' || another == 'y');

5   printf("Exiting...\n");
    return(0);
}

10  void locate(float xx[], unsigned long n, float x, unsigned long *j)
{
    unsigned long ju,jm,jl;
    int ascnd;

15  jl=0;
    ju=n+1;
    ascnd=(xx[n] >= xx[1]);
    while (ju-jl > 1) {
        jm=(ju+jl) » 1;
        if (x >= xx[jm] == ascnd)
            jl=jm;
        else
            ju=jm;
    }
    25  if (x == xx[1])
        *j=1;
    else if (x == xx[n])
        *j=n-1;
    else
        *j=jl;
}

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void norm(float xx[], unsigned long int n)
{
    unsigned long int i;
    float maxdata, temp;

    maxdata = xx[1];
    temp = 0;

    for(i = 2; i <= n; i++) {
        if(xx[i] > maxdata)
            maxdata = xx[i];
    };

    for(i = 1; i <= n; i++) {
        temp = xx[i]/maxdata;
        xx[i] = temp;
    };
}

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5      void baseline(float xx[], unsigned long int n)
     {
     unsigned long int i;
     float mindata, temp;
     mindata = xx [ 1 ] ;
     temp = 0;

10     for(i = 2; i <= n; i++) {
           if(xx[i] < mindata)
               mindata = xx [ i ] ;
     };

15     for(i = 1; i <= n; i++) {
           temp = xx(i) - mindata;
           xx(i) = temp;
     };
     }

```

APPENDIX 3

Program for Determining Strength of Wavelength Response in a Region

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```
#include
<stdio.h>
#include
<stdlib.h>
#include
<math.h>

#define NMAX
3501
#define STRMAX
151
#define FNMAX
81
#define OUTPTS
801

void locate(float xx[], unsigned long n, float x,
unsigned long *j);
void norm(float xx[], unsigned long
int n);
void baseline(float xx[], unsigned
long int n);
void partinteg(float xx[], unsigned long int x1, unsigned long int
x2,
float *area);

int
main()
{
    char fnamein[FNMAX], string[STRMAX], *str_ptr,
fnameout[FNMAX], another;
    float xdata[NMAX], ydata[NMAX], xinter[OUTPTS+1],
yinter[OUTPTS+1];
    float
totalarea,aA,aB,aC,aD,aE,aF,aG,aH,al,aJ,a
K;
    unsigned long int index, i,
j;
    int choice;
    FILE *fpin,
*ffout;
```

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```
another = 'Y';

printf("Contact Rajdeep S. Kalgutkar, SRC-CRC 7-3003, for
further info\n");

do {
    for (i = 0; i <= NMAX-1;
i++) {
        xdata[i]=0;
        ydata[i]=0;
    };

    for (i = 0; i <= OUTPTS;
i++) {
        xinter[i]=0;
        yinter[i]=0;
    };

    printf("\nEnter name of the input file (80 chars max, no
spaces): ");
    scanf("%s",fnamein);

    printf("File name is
%s\n",fnamein);

    fpin =
fopen(fnamein,"r");

    if (fpin ==
NULL) {
        printf("Cannot open %s.
Exiting...\n",fnamein);

        exit(1);
    };

    index = 1;

    while (1) {
        str_ptr = fgets(string,STRMAX-
1,fpin);
        if(str_ptr == NULL)
            break;
        if(index == NMAX)
            break;
        sscanf(string,"%f
%f",&xdata[index],&ydata[index]);
    };
}
```

TO DO LIST

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    index++;
}

fclose(fpin);

if((index == NMAX) && (str_ptr != NULL)) {
    index--;
    printf("Too many data points! Using first %d points
only...\n",index);
}
else {
    index--;
    printf("%d points
read...\n",index);
}

printf("\nEnter option for data
processing\n");
printf("1: Simply interpolate the
data\n");
printf("2: Normalize the data after
interpolation\n");
printf("3: Baseline the data after
interpolation\n");
printf("4: First interpolate, then baseline and finally
");
printf("normalize the
data\n");
printf("or\n");
printf("0: to exit the program without any data
processing\n");
printf("\nEnter option (0-
4): ");
scanf("%d",&choice);

if (choice == 0)

exit(2);

printf("\nEnter name of the output file (80 chars max, no
spaces): ");
scanf("%s",fnameout);

printf("File name is
%s\n",fnameout);

fpout =
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fopen(fnameout,"w");
if (fpout ==
NULL){
    printf("Cannot open %s.
Exiting...\n",fnameout);
exit(3);
};

for(i = 1; i <= OUTPTS;
i++) {
    xinter[i] = 200+((float)i-
1);
    locate(xdata,index,xinter[i],&j);
    if((j == 0) || (j ==
index))
        yinter[i] = 0;
    else
        yinter[i]=(xinter[i]-xdata[j])*((ydata[j+1]-
ydata[j])/
(xdata[j+1]-xdata[j]))+ydata[j];
};

if ((choice == 3) || (choice == 4)) {
baseline(yinter,OUTPTS);
};

if ((choice == 2) || (choice == 4)) {
    norm(yinter,OUTPTS);
};

partinteg(yinter,51,OUTPTS,&totala
rea);

partinteg(yinter,51,101,&a
A);

partinteg(yinter,101,151,&
aB);

partinteg(yinter,151,201,&
aC);

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partinteg(yinter,201,251,&  
aD);  
  
partinteg(yinter,251,301,&  
aE);  
  
partinteg(yinter,301,351,&  
aF);  
  
partinteg(yinter,351,401,&  
aG);  
  
partinteg(yinter,401,451,&  
aH);  
  
partinteg(yinter,451,501,&  
aI);  
  
partinteg(yinter,501,551,&  
aJ);  
  
partinteg(yinter,551,OUTPTS,&aK);  
  
fprintf(fpout,"The total area is:  
%14.6E\n",totalarea);  
fprintf(fpout,"The area under region A is:  
%6.2f%\n",aA*100/totalarea);  
fprintf(fpout,"The area under region B is:  
%6.2f%\n",aB*100/totalarea);  
fprintf(fpout,"The area under region C is:  
%6.2f%\n",aC*100/totalarea);  
fprintf(fpout,"The area under region D is:  
%6.2f%\n",aD*100/totalarea);  
fprintf(fpout,"The area under region E is:  
%6.2f%\n",aE*100/totalarea);  
fprintf(fpout,"The area under region F is:  
%6.2f%\n",aF*100/totalarea);  
fprintf(fpout,"The area under region G is:  
%6.2f%\n",aG*100/totalarea);  
fprintf(fpout,"The area under region H is:  
%6.2f%\n",aH*100/totalarea);  
fprintf(fpout,"The area under region I is:  
%6.2f%\n",aI*100/totalarea);  
fprintf(fpout,"The area under region J is:  
%6.2f%\n",aJ*100/totalarea);  
fprintf(fpout,"The area under region K is:  
%6.2f%\n\n",aK*100/totalarea);
```

```
for (i = 1; i <= OUTPTS-1; i++) {
    fprintf(fpout,"%13.5E, ",yinter[i]);
}
fprintf(fpout,"%13.5E\n",yinter[i]);

fclose(fpout);

printf("File %s
written.\n\n",fnameout);
printf("Process another file
(Y/y/N/n)?: ");
scanf("%1s",&another);
} while (another == 'Y' || another
== 'y');

printf("Exiting...\n
");

return(0
);
}

void locate(float xx[], unsigned long n, float x,
unsigned long *j)
{
    unsigned long ju,jm,jl;
    int ascnd;

    jl=0;

    ju=n+1;
    ascnd=(xx[n] >= xx[1]);
    while (ju-jl > 1) {
        jm=(ju+jl) >> 1;
        if (x >= xx[jm] == ascnd)

            jl=jm;
        else

            ju=jm;
    }
    if (x == xx[1])
        *j=1;
    else if(x ==
```

```

xx[n])
    *j=n-
1;
else
    *j=jl;
}

void norm(float xx[], unsigned long
int n)
{
    unsigned long
int i;
    float maxdata,
temp;

    maxdata =
xx[1];
    temp =
0;

    for(i = 2; i <= n; i++) {
        if(xx[i] >
maxdata)
            maxdata =
xx[i];
    };

    for(i = 1; i <= n; i++) {
        temp = xx[i]/maxdata;
        xx[i] = temp;
    };
}

void baseline(float xx[], unsigned
long int n)
{
    unsigned long
int i;
    float mindata,
temp;

    mindata = xx[1];
    temp =
0;

    for(i = 2; i <= n; i++) {
        if(xx[i] <

```

```
mindata)
    mindata =
xx[i];
};

for(i = 1; i <= n; i++) {
    temp = xx[i] - mindata;
    xx[i] = temp;
};

void partinteg(float xx[], unsigned long int x1, unsigned long int
x2,
    float *area)
{
    unsigned long
int i;
    float temp;

    temp =
0;

    for(i = x1; i <= x2 - 1; i++)
{
    temp = temp + (xx[i] + xx[i+1])/2;
};

    *area = temp;
}
```

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APPENDIX 4

5 Sub Initialize
 Dim ses ses As New NotesSession
 Dim db_db As NotesDatabase
 Dim view view As NotesView
 Dim note_notel As NotesDocument, note_note2 As NotesDocument
 Dim i cnt As Integer, i add As Integer
 10 Set db db =ses ses.CurrentDatabase
 Set note notel=ses ses.DocumentContext
 15 Redim Preserve arr WavelengthRegion(0) air WavelengthRegion(0) _ "
 If note_notel.Selection1(0) <> "" Or rwte_notel.Selection2(0) <> "" Then
 If note notel.Selection1(0) <> "" Then
 Set view_view = db_db.GetView("By NoteID")
 20 If note notel.Selection2(0) <> "" Then
 Set note_note2=view_view.GetDocumentByKey(Right("00000000" &
 note_notel.Selection2(01, 8))
 Else
 25 Set note note2 = view_view.GetDocumentByKey(Right("00000000" &
 note_notel.Selection1(0), \$))
 End If
 30 If Not (note_note2Is Nothing) Then
 If note note2.HasItem("WavelengthRegion") Then
 i_cnt = -1
 Forall vals In note_note2.WavelengthRegion
 If vals <> "" Then
 35 i_cnt = i_cnt + 1
 Redim Preserve arr WavelengthRegion(i_cnt)
 arr_WavelengthRegion(i cnt) = vals
 End If
 End Forall
 40 End If
 End If End If
 45 If note notel.Type(0) = "S" Then
 Set view_View = db_db.GetView("Substrate")
 Elseif note_notel.Type(0) = "P" Then
 Set view_view = db_db.GetView("InitiatorSensitizer") Else
 Set view_view = db_db.GetView("LightSource") End If

```

        ' Set note note2 =view-view. GetFirstDocument

5      i_cnt = -1
      Do While Not (note note2 Is Nothing)
      If note_note2.Name(0) <> "" Then
      L add = True
      If arr WavelengthRegion(0) <> "" Then
      Ladd = False
10     Forall vals1 In note_note2.WavelengthRegion
          Forall vals2 In arr_WavelengthRegion
              If vals1 = vals2 Then
                  i_add = True
                  Exit Forall
15     End If
     End Forall

20     If Ladd Then
          Exit Forall
     End If
     End Forall
     End If

25     If L add Then
          i cnt = i cnt + 1
          Redim Preserve arr_names(i cnt)
          arr names(i cnt) = note_note2.Name(0)
     End If
30     End It
     Set note note2 = view-view. GetNextDocument(note_note2)
     Loop

35     note      _note1 .Names = arr_names
End Sub

SRC Curing Resource dB 4 Query Select2 Save Agent

Sub Initialize
40     Dim ses sesAs New NotesSession
     Dim db_db As NotesDatabase
     Dim view view As NotesView
     Dim note_note1 As NotesDocument, note_note2As NotesDocument

45     Set db_db = ses ses.CurrentDatabase
     Set note note) = ses ses.DocumentContext

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Select Case note_notel.Type(0)
Case "S"
Set view view = db_db.GetView("(Substrate)")
5 Set note_note2=view view.GetDocumentByKey(note_notel.Substrate(0))
Case "P"
Set view=view db-db.GetView("(InitiatorSensitizer)")
10 Set note note2 -view view.GetDocumentByKey(note_notel.Photoinitiator(O))
Case "L"
Set view=view db db.GetView("(LightSource)")
15 Set note_note2 = view_view.GetDocumentByKey(note_notel.LightSource(0))
End Select
20 If note_notel.MexWction(0) = "Add" Then
If note_notel.Selection1 (0) <> "" Then
Print "!" + note_notel.dbname(0) + "/QuerySelection1?OpenForm&" &
note_notel.Selection1 (0) & "&" & note_note2.Noteld & ")"
Else
Print "!" + note_notel.dbname(0) + "/QuerySelection1?OpenForm&" &
note_note2.Noteld & ")"
End If Elseif note_notel.NextAction(0) = "Separate" Then
If note_notel.Selection1(0) <> "" Then
Print "!" + note_notel.dbname(0) + "/QuerySelection1?OpenForm&" &
note_notel.Selection1(O) & "&" & note note2.Noteld & ")"
Else
Print "!" + note_notel.dbname(0) + "/QuerySelection1?OpenForm&" &
note_note2.Noteld & ")"
End If
Elseif note_notel.NextAction(0) = "Separate" Then
If note_notel.Selection2(0) <> "" Then
Print "!" + note_notel.dbname(0) + "/QuerySelectionResults?OpenForm&" &
note_notel.Selection2(0) & _
"&" & note_notel.Selection2(0) & ")"
Elseif note_notel.Selection1(0) <> "" Then
Print "!" + note_notel.dbname(0) + "/QuerySelectionResults?OpenForm&" &
note_notel.Selection1(0) & "&" & note note2.Noteld & ")"
Else
Print "!" + note_notel.dbname(0) + "/QuerySelectionResults?OpenForm&" &
note_notel.Selection1(0) & "&" & note note2.Noteld & ")"
End If
Else
If note_notel.Selection2(0) <> "" Then

```
Print "/" + note_notel.dbname(0) + "/QuerySelectionOverlayResults?OpenForm&" &
note_notel.Selection1(0) & "&" & note_notel.Selection2(0) &
"&" & note_note2.Notelid & ")"
5 Elseif note_notel.Selection1(0) <> "" Then
Print "/" + note_notel.dbname(0) + "/QuerySelectionOverlayResults?OpenForm&" &
note_notel.Selection(0) & "&" & note_note2.Motelid & ")"
Else
Print "/" + note_notel.dbname(0) + "IQuerySelectionOverlayResults?OpenForm&" &
note_note2.Notelid & ")"
10 End If
End If
End Sub
```

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SRC Curing Resource dB 4 Query Overlay Open Agent

Sub Initialize

5 pim ses_ses As New NotesSession
 Dim db db As NotesDatabase
 Dim view-view As NotesView
 Dim note notel As NotesDocument. note_note2As NotesDocument
 Dim i_cntAs Integer, i addAs Integer

10 Set db db = ses.ses.CurrentDatabase
 Set note notel = ses.ses.DocumentContext

15 Set view-view = db_db. GetView("By Note D ")

20 If note notel.Selection1(0) <> "" Then
 Set note-note2 = view-view. GetDocumentByKey(Right("00000000" + note_notel.
 Selection"(0), 8))

25 If Not (note_note2 Is Nothing) Then
 note_notel.data1 = note_note2.EmissData
 note_notel.maxfreq1 = note_note2.MaxFreq
 End If End If

30 If note_notel.Selection2(0) <> "" Then
 Set note-note2 = view_view.GetDocumentByKey(Right("00000000" +
 note_notel.Selection2(0), 8))

35 If Not (note note2 Is Nothing) Then
 note notel.data2=note_note2.EmissData
 note_notel.maxfreq2 = note_note2.MaxFreq
 End If End If

40 If note notel.Selection3(0) <> "" Then
 Set note-note2 = view_view.GetDocumentByKey(Right("00000000" +
 note_notel.Selection3(0), 8))

 If Not (note_note2 Is Nothing) Then
 note notel.data3 = note note2.EmissData
 note_notel.maxfreq3=note note2.MaxFreq
 End If End If End Sub

APPENDIX 5

```
import java.awt.*; import java.awt.event.*; import java.applet.*;  
5  public class SRC Charts extends Applet { int gi count;  
    double GetHMax(String str_in) { String str_current; double dbl hmax;  
10  str_current = ""; dblhmax = 0; for Tint i cnt = 0; i_cnt < str_in.length(); i cnt++) {  
    if(str in. region Match es(i cnt, " ", 0, 2))  
    if(Double.valueOf(str current).doubleValue() > dbl_hmax)  
    dbl hmax = Double.valueOf(str current).doubleValue();  
    str current = " ";  
    i_cnt++;  
15  gi count++; ) else  
    str current = str current.concat(str in.substring(i cnt, i cnt + 1));  
    )  
20  if(str_current.length() > 0) {  
        if(Double.valueOf(str_current).doubleValue() > dbl_hmax)  
        dbl hmax = Double.valueOf(str_current).doubleValue(); gi count++; ) return dbl hmax;  
      
25  int StringToInt(String str_in, double dbl hmax) { double dbl_pos;  
    dbl_pos = getSize().height - (25 + (Double.valueOf(str_in).doubleValue() *  
    ((getSize().height - 50) / dbl hmax))); return (int)dbl-pos; )  
      
30  void drawChartLine(Graphics g, String str_in, String str_type, double dbl_maxfreq) {  
    double dbl_x, dbl_inc, dbl_hmax; String str last, str next;  
    str last str_next = " "; dbl x = 25; gi count = 0;  
    dbl_hmax = GetHMax(str_in); if(str type. equalsIgnoreCase("S")) dbl hmax = 100;  
35  dbl inc = (((double)getSize().width - 50) / gi count) * ((dbl maxfreq - 200) / 800));
```

```

for (int i cnt = 0; i_cnt < str_in.length(); ) “, “, i c{
    nt++if(str_in.regionMatches(i cnt, 0,
5 2))if(str_last.length(> 0) {
    {
g.drawLine((int)dbl x, StringToInt(str_last, dbl hmax), (int)(dbl x + dbl inc),
StringToInt(str_next, dbl hmax));
dbl x = dbl x + dbl inc;

10 str last = str_next; str next = “”; i cnt++;

else { str next = str next.concat(str in.substring(i cnt, i cnt + 1));

)
15 if(str_next.length() > 0)
g.drawLine((int)dbl x, StringToInt(str_last, dbl hmax), (int)(dbl x + dbl-inc),
StringToInt(strnext, dbl_hmax)); }

public void paint(Graphics g) { double dbl x, dbl-y;
20 g.setColor(Color.black); g.drawLine(0, 0, getSize().width, 0); g.drawLine(25,
getSize().height - 25, getSize().width - 25, getSize().height - 25); g.drawLine(25, 25,
25, getSize().height - 25);

25 for(int i cnt = 0; i_cnt < 9; i cnt++) {
    dbl_x = 25 + ((double)i cnt * (((double)getSize().width - 50) / 8));
    g.drawLine((int)dbl x, getSize().height - 25, (int)dbl_x, getSize().height - 20);
    g.drawString(String.valueOf((i cnt * 100) + 200), (int)dbl x - 8, getSize().height - 5); }

30 for(int i cnt = 0; i_cnt < 11; i cnt++) {
    dbl-y = 25 + ((double)i cnt * (((double)getSize().height - 50) / 10));
    g.drawLine(20, (int)dbl-y, 25, (int)dbl-y);
    g.drawString(String.valueOf(100 - (i cnt * 10)), 1, (int)dbl-y + 5); }

35 g.drawString("Data Overlay", (getSize().width / 2) - 30, 12);

g.setColor(Color.red); drawChartLine(g, getParameter("Data 1 "), getParameter("Type
1 "), Double.valueOf(getParameter("Max Freq 1 ")).doubleValue());
g.setColor(Color.blue); drawChartLine(g, getParameter("Data 2"),
40 getParameter("Type 2"), Double.valueOf(getParameter("Max Freq
2")).doubleValue()); g.setColor(Color.green); drawChartLine(g, getParameter("Data
3"), getParameter("Type 3"), Double.valueOf(getParameter("Max Freq
3")).doubleValue()); ) )

```